

Nonequilibrium representative ensembles for isolated quantum systems

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Abstract

An isolated quantum system is considered, prepared in a nonequilibrium initial state. In order to uniquely define the system dynamics, one has to construct a representative statistical ensemble. From the principle of least action it follows that the role of the evolution generator is played by a grand Hamiltonian, but not merely by its energy part. A theorem is proved expressing the commutators of field operators with operator products through variational derivatives of these products. A consequence of this theorem is the equivalence of the variational equations for field operators with the Heisenberg equations for the latter. A finite quantum system cannot equilibrate in the strict sense. But it can tend to a quasi-stationary state characterized by ergodic averages and the appropriate representative ensemble depending on initial conditions. Microcanonical ensemble, arising in the eigenstate thermalization, is just a particular case of representative ensembles. Quasi-stationary representative ensembles are defined by the principle of minimal information. The latter also implies the minimization of an effective thermodynamic potential.

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1 Introduction

Physics of finite quantum systems is now attracting strong attention because of the widespread use of such systems in a variety of applications. As a few examples, it is possible to mention finite spin systems, quantum dots and wells, trapped atoms and ions, and numerous nano- and mesoscopic devices in quantum electronics. Finite systems can be well isolated from

surrounding, which poses several principal questions on the behaviour of isolated quantum systems. Such isolated systems possess the properties that can be essentially different from those of bulk matter typical of condensed-matter materials. Especially difficult is the problem of describing nonequilibrium behaviour of finite quantum systems. Different sides of this problem have been surveyed in reviews [1-8]. One usually studies nonequilibrium effects in particular systems, such as spin assemblies [5,9-18], trapped atoms [4,6,8,14-17], atoms in double wells [18-22], and quantum dots [23].

The aim of the present paper is to analyze several principal problems that are common for the dynamics of many isolated quantum systems prepared in a strongly nonequilibrium initial state. The basic questions that will be studied here are as follows: (i) What is the general rule for constructing nonequilibrium statistical ensembles? (ii) How the variational equations for field operators are connected to the Heisenberg equations of motion? (iii) In what sense an isolated quantum system could equilibrate? The specific feature of the present paper is that the answers to these questions are given not by treating some particular systems but are based on the general principles, such as the principle of least action and the principle of minimal information.

Throughout the paper, the system of units is employed, where the Planck and Boltzmann constants are set to one.

2 Grand Hamiltonian as evolution generator

The behaviour of a nonequilibrium quantum system is characterized by a nonequilibrium quantum ensemble that, by definition, is the pair $\{\mathcal{F}, \hat{\rho}(t)\}$ of the quantum state of microstates \mathcal{F} and a statistical operator $\hat{\rho}(t)$ parametrized by time t . The temporal evolution of the statistical operator is prescribed by the equality

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^+(t) , \quad (1)$$

in which the evolution operator $\hat{U}(t)$ satisfies the Schrödinger equation

$$i \frac{d}{dt} \hat{U}(t) = H\hat{U}(t) , \quad (2)$$

with a Hamiltonian H . This ensemble allows one to get the evolution equations for any observable quantity associated with an operator \hat{A} from an algebra of local observables acting on \mathcal{F} . The measurable quantity is the average

$$\langle \hat{A}(t) \rangle \equiv \text{Tr} \hat{\rho}(t) \hat{A} = \text{Tr} \hat{\rho} \hat{A}(t) , \quad (3)$$

where $\hat{A} \equiv \hat{A}(0)$, $\hat{\rho} \equiv \hat{\rho}(0)$, the trace is over \mathcal{F} , and

$$\hat{A}(t) \equiv \hat{U}^+(t)\hat{A}(0)\hat{U}(t) .$$

Since the dynamics in Eqs. (1) and (2) is generated by the Hamiltonian H , it is termed the *evolution generator*. Thus one comes to the problem of correctly defining the evolution generator, which would make the quantum ensemble completely described. Constructing a statistical ensemble, one must always keep in mind that such an ensemble has to be *representative*, that is, uniquely defining the considered system [24,25]. As was stressed

by Gibbs [26,27], for uniquely characterizing a statistical system, it may be necessary to define not merely an energy operator, but also all those additional constraints that allow for the unique system description. Let \hat{C}_i be self-adjoint operators, enumerated by the index $i = 1, 2, \dots$, whose average values define such *additional conditions*

$$C_i(t) = \langle \hat{C}_i(t) \rangle . \quad (4)$$

A general principle for deriving evolution equations is the principle of least action, or the principle of stationary action. For quantum systems, an action is an operator functional

$$\hat{S} = \int \hat{L}(t) dt , \quad \hat{L}(t) = \hat{E}(t) - \hat{H}(t) , \quad (5)$$

in which $\hat{L}(t)$ is a Lagrangian, with $\hat{E}(t)$ being an energy operator and $\hat{H}(t)$, the energy part of a Hamiltonian. The stationarity of action requires that action (5) be stationary, under the given conditions (4). This is equivalent to the stationarity of the *effective action*

$$S_{eff} = \int \left[\hat{L}(t) - \sum_i \lambda_i \hat{C}_i(t) \right] dt , \quad (6)$$

where λ_i are the Lagrange multipliers guaranteeing the validity of constraints (4). The effective action can be rewritten as

$$S_{eff} = \int \left[\hat{E}(t) - H(t) \right] dt , \quad (7)$$

with the *grand Hamiltonian*

$$H(t) \equiv \hat{H}(t) + \sum_i \lambda_i \hat{C}_i(t) . \quad (8)$$

In this way, to be uniquely defined, preserving all required constraints, the system evolution has to be generated by the grand Hamiltonian (8), but not merely by the energy part \hat{H} .

Let the quantum system be characterized by field operators $\psi(x, t)$, in which x is a set of the variables describing the system. Then the stationarity of action (7) implies the equation

$$\delta S_{eff} = \frac{\delta S_{eff}}{\delta \psi(x, t)} \delta \psi(x, t) + \frac{\delta S_{eff}}{\delta \psi^\dagger(x, t)} \delta \psi^\dagger(x, t) = 0 .$$

With the energy operator

$$\hat{E}(t) = \int \psi^\dagger(x, t) i \frac{\partial}{\partial t} \psi(x, t) dx , \quad (9)$$

one gets the *variational equation*

$$i \frac{\partial}{\partial t} \psi(x, t) = \frac{\delta H(t)}{\delta \psi^\dagger(x, t)} , \quad (10)$$

plus its Hermitian conjugate, playing the role of the Euler-Lagrange equations for quantum systems.

It is important to stress it again that the evolution generator is the grand Hamiltonian (8). Only then the system behavior can be uniquely defined. The internal terms of Hamiltonian (8) do not need to be mutually commutative. That is, the condition operators \hat{C}_i do not have to commute with the energy part \hat{H} . The whole evolution generator H , of course, commutes with itself, hence $H(t) = H$ is an integral of motion.

3 Relation between variational derivatives and commutators

For a quantum system, characterized by field operators, the equations of motion are usually written in the Heisenberg form, where, instead of the variational derivative in Eq. (10), one has a commutator of the field operator with H . One tacitly assumes that these forms should be equivalent, though, to the knowledge of the author, no general proof of this has been given. Here, we prove a very general relation between variational derivatives and commutators, from which the equivalence of the Euler-Lagrange type variational equation (10) and the Heisenberg equation for the field operators follows as a particular case.

The field operators, depending on the particle statistics, satisfy either commutation or anticommutation relations

$$[\psi(x, t), \psi^\dagger(x', t)]_{\mp} = \delta(x - x') , \quad [\psi(x, t), \psi(x', t)]_{\mp} = 0 , \quad (11)$$

in which the upper sign is for Bose and lower, for Fermi statistics. Let the operator

$$\hat{P}_{mn}(t) \equiv P_m^+(t)P_n'(t) \quad (12)$$

be a product of two terms

$$P_m^+(t) \equiv \prod_{i=1}^m \psi^\dagger(x_i, t) , \quad P_n'(t) \equiv \prod_{j=1}^n \psi(x'_j, t) , \quad (13)$$

where m and n are any integers. Then the following proposition is valid.

Theorem 1. For the field operators, satisfying relations (11), the equality is valid:

$$[\psi(x, t), \hat{P}_{mn}(t)] = \frac{\delta \hat{P}_{mn}(t)}{\delta \psi^\dagger(x, t)} + [(\pm 1)^{m+n} - 1] \hat{P}_{mn}(t) \psi(x, t) . \quad (14)$$

Proof. For the left-hand side of Eq. (14), we have

$$[\psi(x, t), \hat{P}_{mn}(t)] = [\psi(x, t), P_m^+(t)] P_n'(t) + P_m^+(t) [\psi(x, t), P_n'(t)] . \quad (15)$$

Here for the first commutator in the right-hand side we find

$$[\psi(x, t), P_m^+(t)] = [(\pm 1)^m - 1] P_m^+(t) \psi(x, t) + \sum_{i=1}^m (\pm 1)^{i+1} \delta(x - x_i) \prod_{j(\neq i)}^m \psi^\dagger(x_j, t) .$$

By definition (12), it is clear that

$$\frac{\delta \hat{P}_{mn}(t)}{\delta \psi^\dagger(x, t)} = \frac{\delta P_m^+(t)}{\delta \psi^\dagger(x, t)} P_n'(t) .$$

Taking the variational derivative, we get

$$\frac{\delta P_m^+(t)}{\delta \psi^\dagger(x, t)} = \sum_{i=1}^m (\pm 1)^{i+1} \delta(x - x_i) \prod_{j(\neq i)}^m \psi^\dagger(x_j, t) .$$

Comparing this with the above commutator gives

$$[\psi(x, t), P_m^+(t)] = \frac{\delta P_m^+(t)}{\delta \psi^\dagger(x, t)} + [(\pm 1)^m - 1] P_m^+(t) \psi(x, t) . \quad (16)$$

Direct calculations also result in

$$[\psi(x, t), P_n'(t)] = [(\pm 1)^n - 1] P_n'(t) \psi(x, t) . \quad (17)$$

Combining Eqs. (15) to (17), we come to relation (14).

An important consequence from this theorem follows for the operators from the algebra of local observables

$$\mathcal{A} \equiv \left\{ \hat{A}(t) \right\} , \quad (18)$$

which are self-adjoint operators possessing the general representation

$$\begin{aligned} \hat{A}(t) = \sum_{mn} \frac{1}{\sqrt{m!n!}} \int A_{mn}(x_1, \dots, x_m; x'_1, \dots, x'_n) \times \\ \times \hat{P}_{mn}(x_1, \dots, x_m; x'_1, \dots, x'_n) dx_1 \dots dx_m dx'_1 \dots dx'_n , \end{aligned} \quad (19)$$

where for Bose statistics m and n in the summation are arbitrary, but for Fermi statistics the summation includes only such m and n for which $m + n$ is even. The latter restriction takes into account the conservation of half-integer spins of fermions. The quantity A_{mn} does not depend on the field operators. The form of \hat{P}_{mn} here is the same as in Eq. (12), but with explicitly shown variables.

Theorem 2. For any operator $\hat{A}(t)$ from the algebra of local observables (18), there exists the relation

$$\left[\psi(x, t), \hat{A}(t) \right] = \frac{\delta \hat{A}(t)}{\delta \psi^\dagger(x, t)} . \quad (20)$$

Proof. Relation (20) is a straightforward consequence of equality (14) for the operators from the algebra of local observables (18).

The system Hamiltonian H pertains to the algebra of local observables (18), hence the right-hand side of the evolution equation (10) coincides with the commutator, according to Eq. (20). That is, the variational equation (10) is equivalent to the Heisenberg equation of motion.

4 Representative ensembles for ergodic averages

The observable quantities (3) can be conveniently rewritten invoking the Hamiltonian basis $\{|n\rangle\}$ defined by the eigenproblem

$$H | n \rangle = E_n | n \rangle . \quad (21)$$

Then the evolution of observables (3), for an isolated quantum system, is given by the equation

$$\langle \hat{A}(t) \rangle = \sum_{mn} \rho_{mn}(t) A_{nm} , \quad (22)$$

where the notation $A_{mn} \equiv \langle m | \hat{A} | n \rangle$ for the matrix elements is used,

$$\rho_{mn}(t) = \rho_{mn}(0) \exp(-i\omega_{mn}t) , \quad (23)$$

and with $\omega_{mn} \equiv E_m - E_n$ being a transition frequency. The normalization condition for the statistical operator becomes

$$\text{Tr} \hat{\rho}(t) = \sum_n \rho_{nn}(t) = 1 . \quad (24)$$

As is evident, the observable quantity (22) is a quasi-periodic function of time. Therefore the limit of observable (22) for t tending to infinity does not exist, and any initial state will be reproduced after the recurrence time that can be estimated [6] as

$$t_{rec} = \frac{2\pi}{\varepsilon N} e^N , \quad (25)$$

where ε is a typical energy per particle. This means that an isolated quantum system cannot equilibrate in the strict sense.

But it may happen that, after the system has been prepared in a nonequilibrium initial state, the observable relaxes close to the ergodic average

$$\overline{\langle \hat{A}(t) \rangle} \equiv \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \langle \hat{A}(t) \rangle dt \quad (26)$$

and stays close to it most of the time, except rare large deviations. Assuming that the spectrum E_n is nondegenerate yields

$$\overline{\langle \hat{A}(t) \rangle} = \sum_n \rho_{nn}(0) A_{nn} . \quad (27)$$

In that case, one can say that the system *quasi-equilibrates* or that it relaxes to a *quasi-equilibrium state* characterized by the ergodic average (27).

Of course, since the ergodic average does not describe a strictly equilibrium state, a finite quantum system may demonstrate large and frequent fluctuations [28]. Then it is not possible to claim that it relaxes to a quasi-equilibrium state. For instance, exactly solvable systems can demonstrate perpetual pulsation for some observables, though showing a kind of relaxation for others [29-31]. Generally, finite quantum systems relax to a quasi-equilibrium state when they are nonintegrable [2-8,32].

As is seen from Eq. (27), the ergodic average depends on the initially prepared state through the value $\rho_{nn}(0)$. If the state, which the system has relaxed to, bears information on initial conditions, then one says that there is no thermalization, since the latter requires some independence from initial conditions.

A trivial case occurs if the initial state is a pure eigenstate $|j\rangle$, when $\rho_{mn} = \delta_{mj}\delta_{nj}$. Then value (22) is strictly stationary: $\langle \hat{A}(t) \rangle = A_{jj}$. That is, if the system initial state is a pure Hamiltonian eigenstate, then there is no any dynamics at all. It is reasonable to assume that, if the initial state is characterized by a weak spread around a fixed pure state, and the system is not integrable, then it would quickly relax to an ergodic average. To concretize this, let us consider a narrow energy shell

$$\mathbb{E}_j \equiv \{E_n : |E_n - E_j| \leq \Delta E_j\} \quad (28)$$

of energies deviating from a given E_j not more then by ΔE_j . And suppose that $\rho_{nn}(0)$ is nonzero only when the related energy E_n is inside shell (28). Assume that this energy shell is so narrow that the matrix elements of the operators of local observables vary a little inside the shell, so that

$$\left| \frac{\Delta A_j}{A_{jj}} \right| \ll 1, \quad \Delta A_j \equiv \max_{E_n \in \mathbb{E}_j} A_{nn} - \min_{E_n \in \mathbb{E}_j} A_{nn}. \quad (29)$$

Then, by the mean value theorem,

$$\sum_{E_n \in \mathbb{E}_j} \rho_{nn}(0) A_{nn} \simeq A_{jj} \sum_{E_n \in \mathbb{E}_j} \rho_{nn}(0) = A_{jj}.$$

The latter equality takes place for any $\rho_{nn}(0)$ normalized according to condition (24). If so, for simplicity, one can accept the uniform expression

$$\rho_{nn}(0) = \frac{1}{Z_j}, \quad Z_j \equiv \sum_{E_n \in \mathbb{E}_j} 1, \quad (30)$$

valid inside shell (28). Summarizing, one has

$$A_{jj} \simeq \sum_{E_n \in \mathbb{E}_j} \rho_{nn}(0) A_{nn} \simeq \frac{1}{Z_j} \sum_{E_n \in \mathbb{E}_j} A_{nn}. \quad (31)$$

Since expression (30) corresponds to a microcanonical distribution, one often terms the resulting Eqs. (31), the eigenstate thermalization hypothesis. However, this is not a hypothesis, as far as Eqs. (31) immediately follow from the assumed conditions (29). What should be called the eigenstate thermalization hypothesis [33,34] would be the assumption that, under the chosen conditions (29), the observable (22) would tend to the ergodic average (27) with the microcanonical distribution (30). This, however, can happen only for nonintegrable systems and for sufficiently narrow energy shell (28) around the energy of an initial stationary state.

More generally, the initial value $\rho_{nn}(0)$ can be characterized by a representative ensemble uniquely defining the considered system. For this purpose, one can invoke the maximization of entropy under the given additional constraints [35-37], which is equivalent to the minimization of the information functional [38,39]. Formulating the additional constraints as in Eq. (4), with explicitly separating the condition for the internal energy E , we have the information functional

$$I[\hat{\rho}] = \text{Tr} \hat{\rho} \ln \hat{\rho} + \lambda_0 (\text{Tr} \hat{\rho} - 1) + \beta (\text{Tr} \hat{\rho} \hat{H} - E) + \beta \sum_i \lambda_i (\text{Tr} \hat{\rho} \hat{C}_i - C_i), \quad (32)$$

where λ_0, β , and λ_i are the Lagrange multipliers. Minimizing the information functional (32) yields

$$\hat{\rho} = \frac{1}{Z} e^{-\beta H}, \quad Z \equiv \text{Tr} e^{-\beta H}, \quad (33)$$

with the same grand Hamiltonian (8) that generates the system dynamics. Due to expression (33), we have

$$\rho_{nn}(0) = \frac{1}{Z} e^{-\beta E_n}. \quad (34)$$

The Lagrange multipliers $\beta = \beta(E, C_1, C_2, \dots)$ and $\lambda_i = \lambda_i(E, C_1, C_2, \dots)$ are defined through the given values of observables E and C_i by the equations

$$\text{Tr} \hat{\rho} \hat{H} = E, \quad \text{Tr} \hat{\rho} \hat{C}_i = C_i.$$

The microcanonical distribution (30) is a particular case of distribution (34) under $\beta \rightarrow 0$.

The pair $\{\mathcal{F}, \hat{\rho}\}$, with the statistical operator (33), forms a representative ensemble describing the quasi-equilibrium state which a finite quantum system equilibrates to. As is evident, this ensemble is defined by invoking the information on the diagonal elements of $\rho_{nn}(0)$ at the initial moment of time. As has been stressed above, the necessity of taking into account all constraints uniquely defining the system, composing a grand Hamiltonian (8), was emphasized by Gibbs [26,27]. The term *representative ensemble* was used by Tolman [24] and ter Haar [25]. The derivation of the statistical operator by maximizing entropy, under the given constraints, was advanced by Shannon [35,36] and later advocated by Janes [37]. One sometimes calls the representative ensembles as generalized, or conditional, Gibbs ensembles. But one should not forget that such grand ensembles were introduced by Gibbs. Representative ensembles can be defined for stationary as well as nonstationary systems [38-43]. More details and an extensive list of references can be found in review [6].

If the statistical operator (33) depends on some unspecified parameters or functions, these can be specified by minimizing the information functional (32). Substituting expression (33) into functional (32) gives

$$I[\hat{\rho}] = \beta(\Omega - E), \quad \Omega \equiv -T \ln Z, \quad (35)$$

where Ω is the grand thermodynamic potential. Since the value E here is fixed, the minimization of the information functional is equivalent to the minimization of the thermodynamic potential:

$$\min I[\hat{\rho}] \longleftrightarrow \min \Omega.$$

In this way, when a finite quantum system equilibrates to a quasi-equilibrium state, the latter is described by a representative ensemble, whose definition is based on the information on the initially prepared state. Of special importance is the prescription of the initial state symmetry when the dynamics of a finite system involves the creation of topological defects [4,44,45].

5 Conclusion

The evolution of a finite quantum system is considered, starting from a nonequilibrium initial state. Being based on the principle of least action, it is shown that the system evolution is generated by a grand Hamiltonian. This defines a nonequilibrium representative ensemble, taking into account all constraints required for the unique system description.

A theorem is proved expressing the commutators of field operators with the operator products through variational derivatives of the latter. Using this theorem, it is proved that the variation of the operators from the algebra of local observables is related to the commutators of these observables with field operators. The variational evolution equations, playing the role of the quantum Euler-Lagrange equations, are shown to be equivalent to the Heisenberg equations of motion.

A finite quantum system cannot equilibrate in the strict sense. But it can tend to a quasi-stationary state corresponding to the ergodic averages. This state exists in the time interval between the relaxation time and the recurrence time. The resulting quasi-stationary states are characterized by representative ensembles, whose definition involves information on the initially prepared state of the system. Microcanonical ensemble is a particular case of representative ensembles. Generally, such representative ensembles are defined by minimizing the appropriate information functionals. The minimum of the latter also implies the minimum of the related thermodynamic potential.

Strictly speaking, equilibration requires that all system observables would relax to their quasi-stationary values. Relaxation times for different observables can be different. Integrable systems can display relaxation for some observables but the absence of such a relaxation for others. Nonintegrable systems always relax to quasi-stationary states described by representative quantum ensembles.

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